



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 07:59 PM UTC

PDB ID : 5K0T / pdb_00005k0t
Title : Crystal structure of methionyl-tRNA synthetase MetRS from Brucella melitensis in complex with inhibitor Chem 1415
Authors : Seattle Structural Genomics Center for Infectious Disease (SSGCID)
Deposited on : 2016-05-17
Resolution : 2.60 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

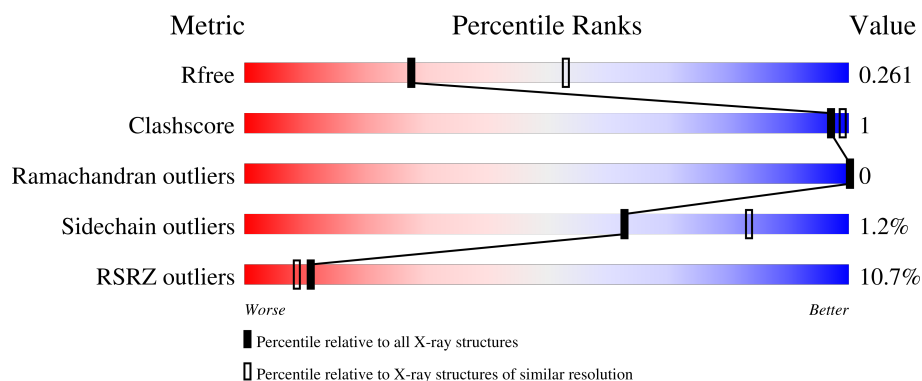
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.60 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	4008 (2.60-2.60)
Clashscore	190562	4347 (2.60-2.60)
Ramachandran outliers	187476	4277 (2.60-2.60)
Sidechain outliers	187428	4277 (2.60-2.60)
RSRZ outliers	180081	4008 (2.60-2.60)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	536	11% 89% 7%
1	B	536	5% 84% 13%
1	C	536	13% 87% 10%

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 11462 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a protein called Methionine-tRNA ligase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	496	Total	C	N	O	S	0	2	0
			3850	2454	662	720	14			
1	B	468	Total	C	N	O	S	0	0	0
			3640	2326	625	675	14			
1	C	481	Total	C	N	O	S	0	2	0
			3699	2362	633	689	15			

There are 66 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-20	MET	-	initiating methionine	UNP P59078
A	-19	ALA	-	expression tag	UNP P59078
A	-18	HIS	-	expression tag	UNP P59078
A	-17	HIS	-	expression tag	UNP P59078
A	-16	HIS	-	expression tag	UNP P59078
A	-15	HIS	-	expression tag	UNP P59078
A	-14	HIS	-	expression tag	UNP P59078
A	-13	HIS	-	expression tag	UNP P59078
A	-12	MET	-	expression tag	UNP P59078
A	-11	GLY	-	expression tag	UNP P59078
A	-10	THR	-	expression tag	UNP P59078
A	-9	LEU	-	expression tag	UNP P59078
A	-8	GLU	-	expression tag	UNP P59078
A	-7	ALA	-	expression tag	UNP P59078
A	-6	GLN	-	expression tag	UNP P59078
A	-5	THR	-	expression tag	UNP P59078
A	-4	GLN	-	expression tag	UNP P59078
A	-3	GLY	-	expression tag	UNP P59078
A	-2	PRO	-	expression tag	UNP P59078
A	-1	GLY	-	expression tag	UNP P59078
A	0	SER	-	expression tag	UNP P59078
A	70	ASP	GLU	conflict	UNP P59078
B	-20	MET	-	initiating methionine	UNP P59078

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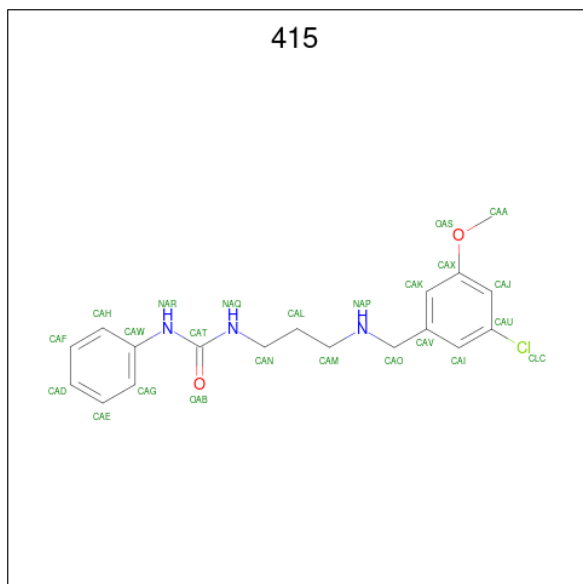
Chain	Residue	Modelled	Actual	Comment	Reference
B	-19	ALA	-	expression tag	UNP P59078
B	-18	HIS	-	expression tag	UNP P59078
B	-17	HIS	-	expression tag	UNP P59078
B	-16	HIS	-	expression tag	UNP P59078
B	-15	HIS	-	expression tag	UNP P59078
B	-14	HIS	-	expression tag	UNP P59078
B	-13	HIS	-	expression tag	UNP P59078
B	-12	MET	-	expression tag	UNP P59078
B	-11	GLY	-	expression tag	UNP P59078
B	-10	THR	-	expression tag	UNP P59078
B	-9	LEU	-	expression tag	UNP P59078
B	-8	GLU	-	expression tag	UNP P59078
B	-7	ALA	-	expression tag	UNP P59078
B	-6	GLN	-	expression tag	UNP P59078
B	-5	THR	-	expression tag	UNP P59078
B	-4	GLN	-	expression tag	UNP P59078
B	-3	GLY	-	expression tag	UNP P59078
B	-2	PRO	-	expression tag	UNP P59078
B	-1	GLY	-	expression tag	UNP P59078
B	0	SER	-	expression tag	UNP P59078
B	70	ASP	GLU	conflict	UNP P59078
C	-20	MET	-	initiating methionine	UNP P59078
C	-19	ALA	-	expression tag	UNP P59078
C	-18	HIS	-	expression tag	UNP P59078
C	-17	HIS	-	expression tag	UNP P59078
C	-16	HIS	-	expression tag	UNP P59078
C	-15	HIS	-	expression tag	UNP P59078
C	-14	HIS	-	expression tag	UNP P59078
C	-13	HIS	-	expression tag	UNP P59078
C	-12	MET	-	expression tag	UNP P59078
C	-11	GLY	-	expression tag	UNP P59078
C	-10	THR	-	expression tag	UNP P59078
C	-9	LEU	-	expression tag	UNP P59078
C	-8	GLU	-	expression tag	UNP P59078
C	-7	ALA	-	expression tag	UNP P59078
C	-6	GLN	-	expression tag	UNP P59078
C	-5	THR	-	expression tag	UNP P59078
C	-4	GLN	-	expression tag	UNP P59078
C	-3	GLY	-	expression tag	UNP P59078
C	-2	PRO	-	expression tag	UNP P59078
C	-1	GLY	-	expression tag	UNP P59078
C	0	SER	-	expression tag	UNP P59078

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Chain	Residue	Modelled	Actual	Comment	Reference
C	70	ASP	GLU	conflict	UNP P59078

- Molecule 2 is 1-{3-[(3-chloro-5-methoxybenzyl)amino]propyl}-3-phenylurea (CCD ID: 415) (formula: C₁₈H₂₂ClN₃O₂).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	Cl	N	O	0	0
			24	18	1	3	2		
2	B	1	Total	C	Cl	N	O	0	0
			24	18	1	3	2		
2	C	1	Total	C	Cl	N	O	0	0
			24	18	1	3	2		

- Molecule 3 is 1,2-ETHANEDIOL (CCD ID: EDO) (formula: C₂H₆O₂).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	1	Total C O 4 2 2	0	0
3	A	1	Total C O 4 2 2	0	0
3	A	1	Total C O 4 2 2	0	0
3	A	1	Total C O 4 2 2	0	0
3	B	1	Total C O 4 2 2	0	0
3	B	1	Total C O 4 2 2	0	0
3	B	1	Total C O 4 2 2	0	0
3	C	1	Total C O 4 2 2	0	0

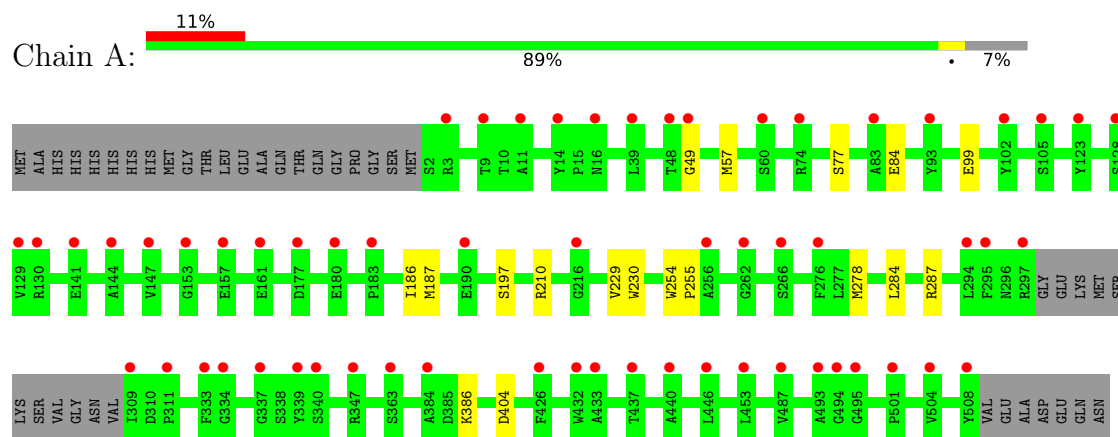
- Molecule 4 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	52	Total O 52 52	0	0
4	B	69	Total O 69 69	0	0
4	C	48	Total O 48 48	0	0

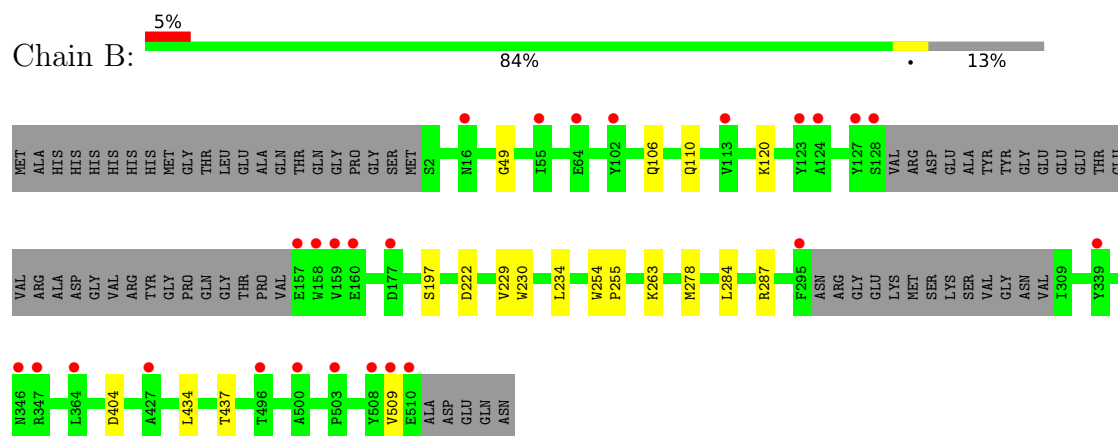
3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density ($RSRZ > 2$). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

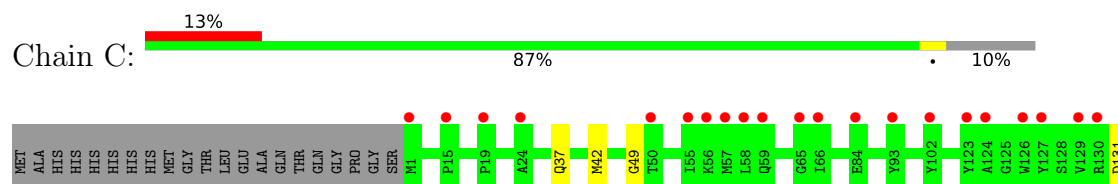
• Molecule 1: Methionine-tRNA ligase

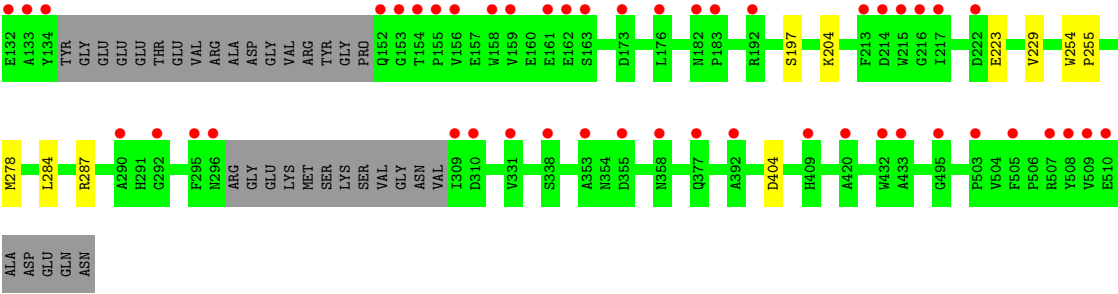


• Molecule 1: Methionine-tRNA ligase



• Molecule 1: Methionine-tRNA ligase





4 Data and refinement statistics

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α , β , γ	45.16Å 99.65Å 104.30Å 110.46° 88.09° 99.72°	Depositor
Resolution (Å)	50.00 – 2.60 50.00 – 2.60	Depositor EDS
% Data completeness (in resolution range)	96.1 (50.00-2.60) 96.1 (50.00-2.60)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.17 (at 2.61Å)	Xtriage
Refinement program	REFMAC	Depositor
R, R_{free}	0.257 , 0.286 (Not available) , 0.261	Depositor DCC
R_{free} test set	2416 reflections (4.68%)	wwPDB-VP
Wilson B-factor (Å ²)	46.7	Xtriage
Anisotropy	0.468	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.31 , 29.1	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.88	EDS
Total number of atoms	11462	wwPDB-VP
Average B, all atoms (Å ²)	51.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.38% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: EDO, 415

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
1	A	0.59	0/3958	0.86	2/5400 (0.0%)
1	B	0.58	0/3735	0.84	2/5090 (0.0%)
1	C	0.59	0/3799	0.86	2/5179 (0.0%)
All	All	0.59	0/11492	0.86	6/15669 (0.0%)

There are no bond length outliers.

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	57	MET	CG-SD-CE	-5.73	88.29	100.90
1	A	49	GLY	N-CA-C	5.48	118.25	110.74
1	C	229	VAL	N-CA-C	5.48	116.87	110.62
1	B	49	GLY	N-CA-C	5.23	117.90	110.74
1	C	49	GLY	N-CA-C	5.17	117.82	110.74
1	B	229	VAL	N-CA-C	5.14	116.48	110.62

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3850	0	3610	7	0
1	B	3640	0	3449	8	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	C	3699	0	3502	4	0
2	A	24	0	22	3	0
2	B	24	0	22	2	0
2	C	24	0	22	0	0
3	A	16	0	24	0	0
3	B	12	0	18	0	0
3	C	4	0	6	0	0
4	A	52	0	0	0	0
4	B	69	0	0	0	0
4	C	48	0	0	0	0
All	All	11462	0	10675	19	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 1.

All (19) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:186:ILE:O	1:A:187:MET:HE2	1.93	0.68
1:A:230:TRP:HE3	2:A:601:415:H1	1.70	0.57
1:A:278:MET:HE3	1:A:284:LEU:HD21	1.94	0.50
1:C:278:MET:HE3	1:C:284:LEU:HD21	1.95	0.49
1:A:230:TRP:CE3	2:A:601:415:H1	2.47	0.49
1:B:230:TRP:HE3	2:B:601:415:H1	1.78	0.49
1:A:229:VAL:HG22	2:A:601:415:H3	1.96	0.48
1:B:234:LEU:HG	2:B:601:415:H3	1.96	0.47
1:B:278:MET:HE3	1:B:284:LEU:HD21	1.95	0.47
1:B:287:ARG:NH1	1:B:404:ASP:O	2.48	0.47
1:A:287:ARG:NH1	1:A:404:ASP:O	2.48	0.46
1:B:120:LYS:HE3	1:B:222:ASP:OD2	2.14	0.46
1:B:254:TRP:CD2	1:B:255:PRO:HA	2.51	0.45
1:A:254:TRP:CD2	1:A:255:PRO:HA	2.51	0.45
1:C:287:ARG:NH1	1:C:404:ASP:O	2.49	0.45
1:B:434:LEU:HA	1:B:437:THR:OG1	2.17	0.44
1:C:254:TRP:CD2	1:C:255:PRO:HA	2.52	0.44
1:C:37:GLN:HE21	1:C:42:MET:HG3	1.85	0.42
1:B:106:GLN:O	1:B:110:GLN:HG2	2.21	0.40

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	494/536 (92%)	486 (98%)	8 (2%)	0	100	100
1	B	462/536 (86%)	457 (99%)	5 (1%)	0	100	100
1	C	477/536 (89%)	471 (99%)	6 (1%)	0	100	100
All	All	1433/1608 (89%)	1414 (99%)	19 (1%)	0	100	100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	378/437 (86%)	372 (98%)	6 (2%)	55	79
1	B	361/437 (83%)	358 (99%)	3 (1%)	73	88
1	C	366/437 (84%)	362 (99%)	4 (1%)	65	84
All	All	1105/1311 (84%)	1092 (99%)	13 (1%)	63	83

All (13) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	77	SER
1	A	84	GLU
1	A	99	GLU
1	A	197	SER
1	A	210	ARG

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Mol	Chain	Res	Type
1	A	386	LYS
1	B	197	SER
1	B	263	LYS
1	B	509	VAL
1	C	131	ASP
1	C	197	SER
1	C	204	LYS
1	C	223	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (6) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	37	GLN
1	A	182	ASN
1	B	23	HIS
1	C	37	GLN
1	C	354	ASN
1	C	361	GLN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains [i](#)

There are no non-standard protein/DNA/RNA residues in this entry.

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

11 ligands are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond

length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	415	B	601	-	25,25,25	2.10	10 (40%)	31,31,31	0.95	1 (3%)
3	EDO	B	603	-	3,3,3	0.46	0	2,2,2	0.28	0
2	415	C	601	-	25,25,25	2.09	9 (36%)	31,31,31	0.98	2 (6%)
3	EDO	A	604	-	3,3,3	0.44	0	2,2,2	0.32	0
3	EDO	A	602	-	3,3,3	0.43	0	2,2,2	0.33	0
2	415	A	601	-	25,25,25	2.08	10 (40%)	31,31,31	1.03	3 (9%)
3	EDO	A	605	-	3,3,3	0.43	0	2,2,2	0.33	0
3	EDO	B	604	-	3,3,3	0.44	0	2,2,2	0.33	0
3	EDO	B	602	-	3,3,3	0.43	0	2,2,2	0.36	0
3	EDO	A	603	-	3,3,3	0.45	0	2,2,2	0.31	0
3	EDO	C	602	-	3,3,3	0.43	0	2,2,2	0.34	0

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	415	B	601	-	-	5/15/15/15	0/2/2/2
3	EDO	B	603	-	-	1/1/1/1	-
2	415	C	601	-	-	4/15/15/15	0/2/2/2
3	EDO	A	604	-	-	0/1/1/1	-
3	EDO	A	602	-	-	0/1/1/1	-
2	415	A	601	-	-	6/15/15/15	0/2/2/2
3	EDO	A	605	-	-	1/1/1/1	-
3	EDO	B	604	-	-	1/1/1/1	-
3	EDO	B	602	-	-	1/1/1/1	-
3	EDO	A	603	-	-	1/1/1/1	-
3	EDO	C	602	-	-	1/1/1/1	-

All (29) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	C	601	415	CAT-NAR	4.25	1.46	1.37
2	A	601	415	CAT-NAR	4.20	1.46	1.37
2	B	601	415	CAT-NAR	4.19	1.46	1.37
2	C	601	415	CAT-NAQ	3.97	1.43	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	601	415	CAT-NAQ	3.77	1.42	1.35
2	B	601	415	CAT-NAQ	3.60	1.42	1.35
2	A	601	415	CAE-CAG	3.45	1.44	1.38
2	B	601	415	CAE-CAG	3.45	1.44	1.38
2	C	601	415	CAK-CAV	3.34	1.45	1.39
2	B	601	415	CAK-CAV	3.32	1.44	1.39
2	C	601	415	CAE-CAG	3.25	1.44	1.38
2	A	601	415	CAK-CAV	3.20	1.44	1.39
2	B	601	415	CAJ-CAX	2.99	1.43	1.39
2	C	601	415	CAJ-CAX	2.81	1.43	1.39
2	B	601	415	CAI-CAU	2.74	1.42	1.38
2	C	601	415	CAI-CAU	2.74	1.42	1.38
2	A	601	415	CAJ-CAX	2.74	1.43	1.39
2	C	601	415	CAH-CAW	2.73	1.43	1.39
2	A	601	415	CAI-CAU	2.66	1.42	1.38
2	B	601	415	CAN-NAQ	-2.63	1.40	1.46
2	A	601	415	CAH-CAW	2.59	1.43	1.39
2	B	601	415	CAH-CAW	2.56	1.43	1.39
2	A	601	415	CAN-NAQ	-2.52	1.40	1.46
2	C	601	415	CAN-NAQ	-2.52	1.40	1.46
2	A	601	415	CAF-CAH	2.13	1.42	1.38
2	B	601	415	CAF-CAH	2.08	1.42	1.38
2	A	601	415	CAL-CAM	2.05	1.59	1.51
2	B	601	415	CAL-CAM	2.04	1.59	1.51
2	C	601	415	CAL-CAM	2.03	1.59	1.51

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	601	415	CAA-OAS-CAX	-2.60	111.93	117.50
2	B	601	415	CAI-CAU-CLC	2.51	122.32	119.17
2	A	601	415	NAR-CAT-NAQ	2.41	117.85	113.83
2	C	601	415	CAI-CAU-CLC	2.11	121.81	119.17
2	A	601	415	CAI-CAU-CLC	2.09	121.79	119.17
2	C	601	415	NAR-CAT-NAQ	2.04	117.24	113.83

There are no chirality outliers.

All (21) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	601	415	CAK-CAX-OAS-CAA
2	A	601	415	CAJ-CAX-OAS-CAA

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Mol	Chain	Res	Type	Atoms
2	C	601	415	CAJ-CAX-OAS-CAA
2	C	601	415	CAK-CAX-OAS-CAA
2	B	601	415	CAJ-CAX-OAS-CAA
2	B	601	415	CAK-CAX-OAS-CAA
2	A	601	415	CAN-CAL-CAM-NAP
2	B	601	415	CAV-CAO-NAP-CAM
2	B	601	415	CAN-CAL-CAM-NAP
2	A	601	415	CAV-CAO-NAP-CAM
2	C	601	415	CAL-CAM-NAP-CAO
2	B	601	415	CAM-CAL-CAN-NAQ
2	C	601	415	CAN-CAL-CAM-NAP
3	A	603	EDO	O1-C1-C2-O2
3	C	602	EDO	O1-C1-C2-O2
2	A	601	415	CAM-CAL-CAN-NAQ
3	B	602	EDO	O1-C1-C2-O2
3	A	605	EDO	O1-C1-C2-O2
3	B	603	EDO	O1-C1-C2-O2
3	B	604	EDO	O1-C1-C2-O2
2	A	601	415	CAL-CAM-NAP-CAO

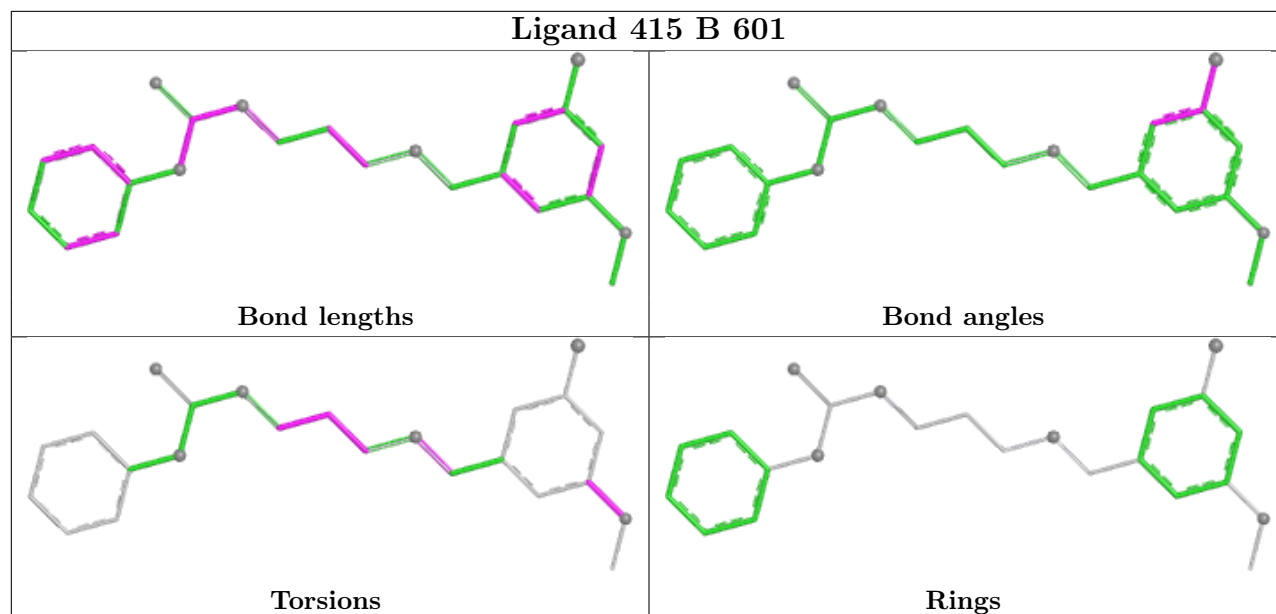
There are no ring outliers.

2 monomers are involved in 5 short contacts:

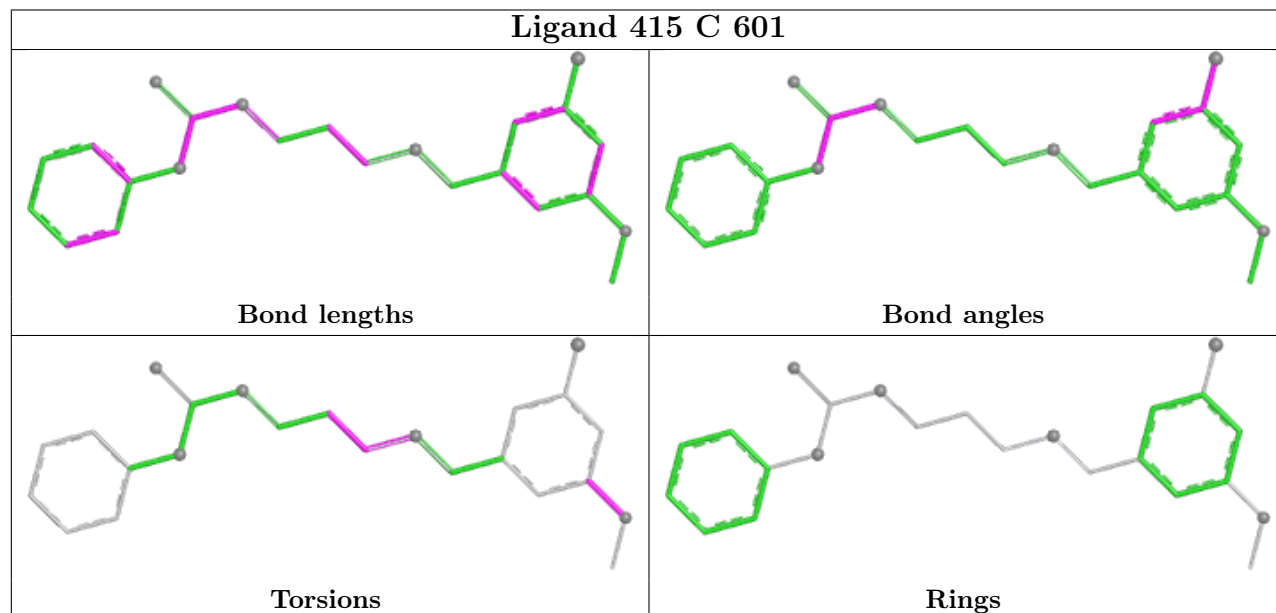
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	B	601	415	2	0
2	A	601	415	3	0

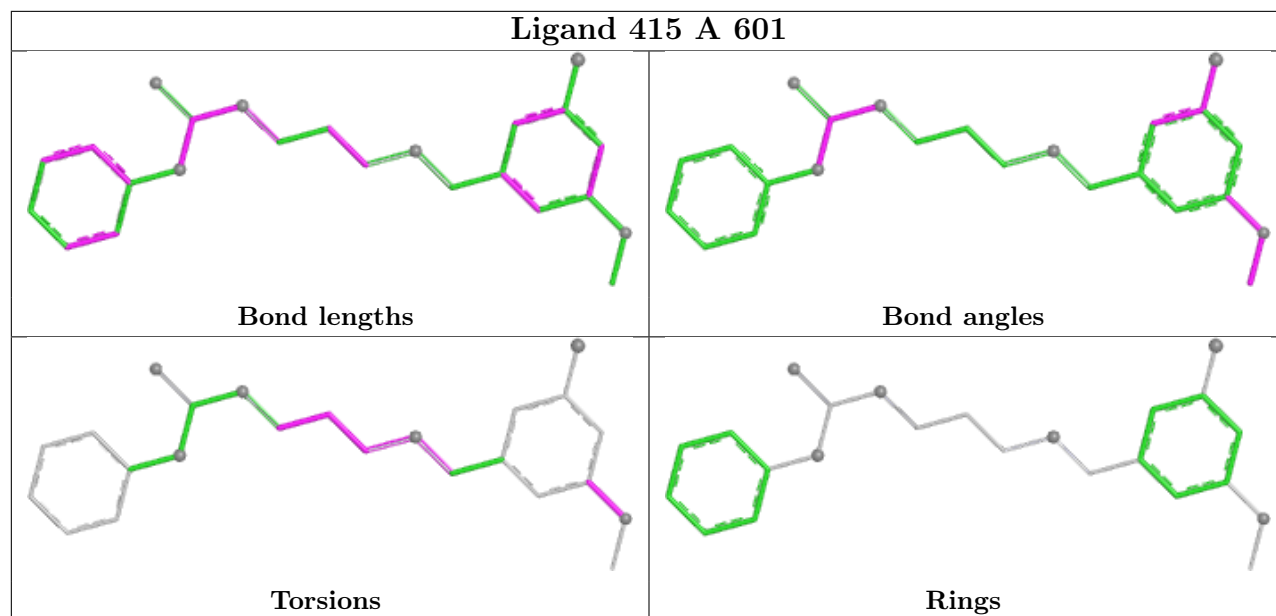
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.

Ligand 415 B 601



Ligand 415 C 601





5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

In the following table, the column labelled ‘#RSRZ > 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q < 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	496/536 (92%)	1.11	60 (12%) 8 6	27, 52, 69, 81	2 (0%)
1	B	468/536 (87%)	0.93	26 (5%) 30 24	32, 45, 59, 121	0
1	C	481/536 (89%)	1.19	69 (14%) 6 5	33, 51, 76, 136	2 (0%)
All	All	1445/1608 (89%)	1.08	155 (10%) 11 9	27, 49, 70, 136	4 (0%)

All (155) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	134	TYR	5.3
1	B	128	SER	5.0
1	C	55	ILE	4.7
1	C	133	ALA	4.4
1	C	132	GLU	4.4
1	A	144	ALA	4.2
1	B	160	GLU	4.1
1	B	157	GLU	4.0
1	C	153	GLY	3.8
1	C	173	ASP	3.8
1	C	331	VAL	3.8
1	A	16	ASN	3.7
1	C	510	GLU	3.7
1	C	296	ASN	3.7
1	C	124	ALA	3.6
1	B	127	TYR	3.6
1	C	126	TRP	3.6
1	C	154	THR	3.3
1	C	156	VAL	3.3
1	C	1	MET	3.2
1	B	64	GLU	3.2
1	A	123	TYR	3.2
1	C	127	TYR	3.2

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Mol	Chain	Res	Type	RSRZ
1	C	509	VAL	3.2
1	C	155	PRO	3.1
1	B	339	TYR	3.1
1	A	177	ASP	3.1
1	A	105	SER	3.1
1	B	346	ASN	3.1
1	B	509	VAL	3.0
1	C	58	LEU	3.0
1	C	66	ILE	3.0
1	C	290	ALA	3.0
1	B	16	ASN	2.9
1	C	215	TRP	2.9
1	A	494	GLY	2.9
1	C	377	GLN	2.9
1	C	130	ARG	2.9
1	A	334	GLY	2.9
1	B	124	ALA	2.9
1	C	158	TRP	2.8
1	C	216	GLY	2.8
1	B	500	ALA	2.8
1	C	213	PHE	2.8
1	A	294	LEU	2.8
1	C	353	ALA	2.8
1	C	65	GLY	2.8
1	C	433	ALA	2.8
1	A	102	TYR	2.8
1	A	60	SER	2.7
1	A	266	SER	2.7
1	B	158	TRP	2.7
1	A	432	TRP	2.7
1	C	123	TYR	2.7
1	A	347[A]	ARG	2.7
1	A	495	GLY	2.7
1	A	3	ARG	2.6
1	A	161	GLU	2.6
1	A	311	PRO	2.6
1	B	159	VAL	2.6
1	A	9	THR	2.6
1	A	11	ALA	2.6
1	A	129	VAL	2.6
1	A	384	ALA	2.6
1	C	432	TRP	2.6

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Mol	Chain	Res	Type	RSRZ
1	C	57	MET	2.6
1	A	508	TYR	2.6
1	C	161	GLU	2.6
1	A	130	ARG	2.5
1	A	183	PRO	2.5
1	A	493	ALA	2.5
1	C	217	ILE	2.5
1	A	262	GLY	2.5
1	A	433	ALA	2.5
1	C	295	PHE	2.5
1	C	214	ASP	2.4
1	B	102	TYR	2.4
1	A	147	VAL	2.4
1	C	222	ASP	2.4
1	C	162	GLU	2.4
1	C	19	PRO	2.4
1	B	295	PHE	2.4
1	C	503	PRO	2.4
1	C	310	ASP	2.4
1	B	177	ASP	2.3
1	A	49	GLY	2.3
1	A	157	GLU	2.3
1	A	180	GLU	2.3
1	A	501	PRO	2.3
1	C	507	ARG	2.3
1	C	508	TYR	2.3
1	C	15	PRO	2.3
1	A	39	LEU	2.3
1	A	83	ALA	2.3
1	A	437	THR	2.3
1	A	14	TYR	2.3
1	A	339	TYR	2.3
1	B	508	TYR	2.3
1	C	84	GLU	2.3
1	B	503	PRO	2.3
1	B	364	LEU	2.3
1	C	129	VAL	2.3
1	A	440	ALA	2.2
1	A	153	GLY	2.2
1	C	420	ALA	2.2
1	C	338	SER	2.2
1	B	510	GLU	2.2

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Mol	Chain	Res	Type	RSRZ
1	C	59	GLN	2.2
1	A	504	VAL	2.2
1	A	141	GLU	2.2
1	A	297	ARG	2.2
1	B	347	ARG	2.2
1	A	453	LEU	2.2
1	A	216	GLY	2.1
1	A	363	SER	2.1
1	A	487	VAL	2.1
1	C	409	HIS	2.1
1	A	256	ALA	2.1
1	C	24	ALA	2.1
1	C	192	ARG	2.1
1	C	50	THR	2.1
1	C	183	PRO	2.1
1	B	55	ILE	2.1
1	C	309	ILE	2.1
1	C	355	ASP	2.1
1	A	295	PHE	2.1
1	C	163	SER	2.1
1	B	496	THR	2.1
1	C	358	ASN	2.1
1	A	93	TYR	2.1
1	B	123	TYR	2.1
1	A	426	PHE	2.1
1	A	74	ARG	2.1
1	A	190	GLU	2.1
1	B	427	ALA	2.1
1	C	56	LYS	2.1
1	A	48	THR	2.1
1	C	152	GLN	2.1
1	C	182[A]	ASN	2.1
1	A	309	ILE	2.1
1	C	102	TYR	2.1
1	C	159	VAL	2.1
1	A	276	PHE	2.1
1	C	505	PHE	2.1
1	A	128	SER	2.0
1	A	340	SER	2.0
1	A	446	LEU	2.0
1	A	333	PHE	2.0
1	C	392	ALA	2.0

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Mol	Chain	Res	Type	RSRZ
1	C	176	LEU	2.0
1	A	337	GLY	2.0
1	C	292	GLY	2.0
1	C	495	GLY	2.0
1	B	113	VAL	2.0
1	C	93	TYR	2.0

6.2 Non-standard residues in protein, DNA, RNA chains [i](#)

There are no non-standard protein/DNA/RNA residues in this entry.

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

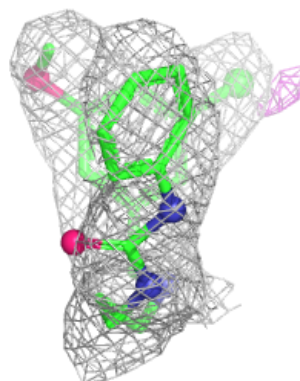
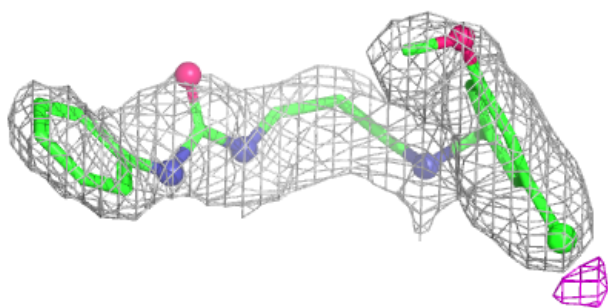
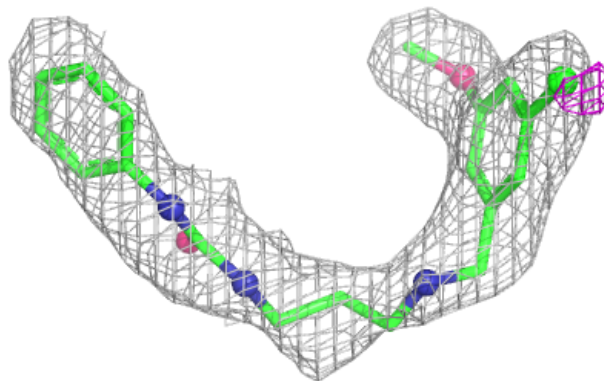
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
3	EDO	C	602	4/4	0.63	0.18	79,80,80,80	0
3	EDO	B	602	4/4	0.67	0.20	71,72,72,72	0
3	EDO	A	604	4/4	0.67	0.20	72,72,72,72	0
3	EDO	B	603	4/4	0.71	0.30	68,68,68,68	0
3	EDO	A	602	4/4	0.72	0.18	56,56,57,57	0
3	EDO	A	605	4/4	0.73	0.19	82,83,83,83	0
3	EDO	A	603	4/4	0.79	0.15	58,58,58,58	0
3	EDO	B	604	4/4	0.80	0.20	76,76,76,77	0
2	415	A	601	24/24	0.80	0.19	54,59,61,62	0
2	415	C	601	24/24	0.83	0.17	50,59,63,65	0
2	415	B	601	24/24	0.86	0.16	47,52,58,62	0

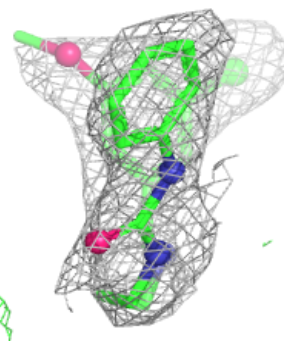
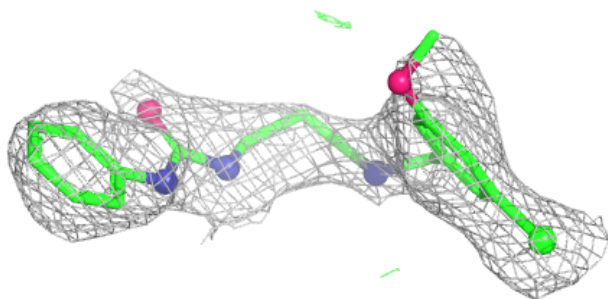
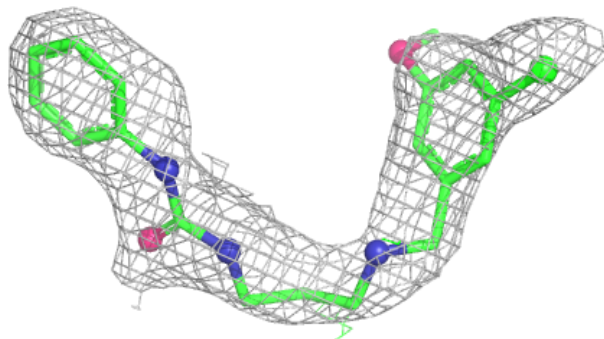
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation to approximate a three-dimensional view.

Electron density around 415 A 601:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

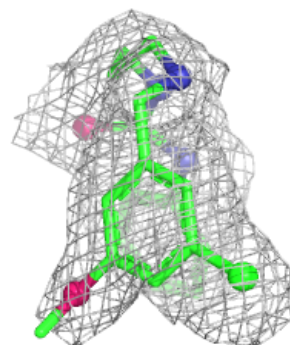
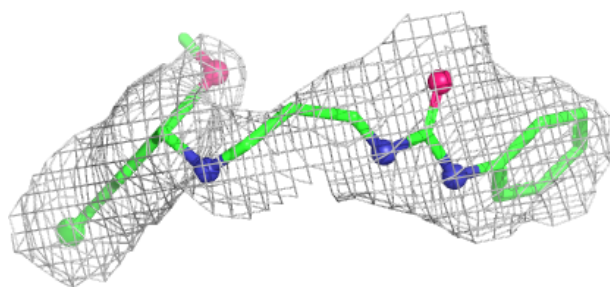
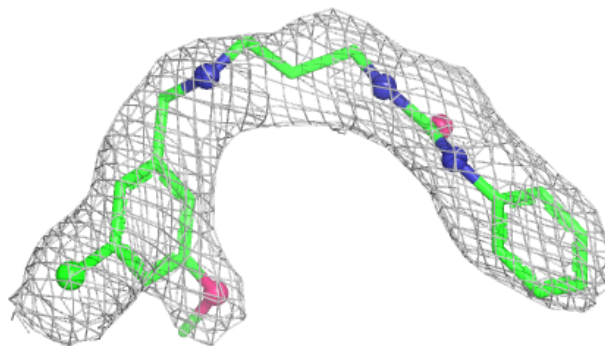
**Electron density around 415 C 601:**

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



Electron density around 415 B 601:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



6.5 Other polymers [i](#)

There are no such residues in this entry.